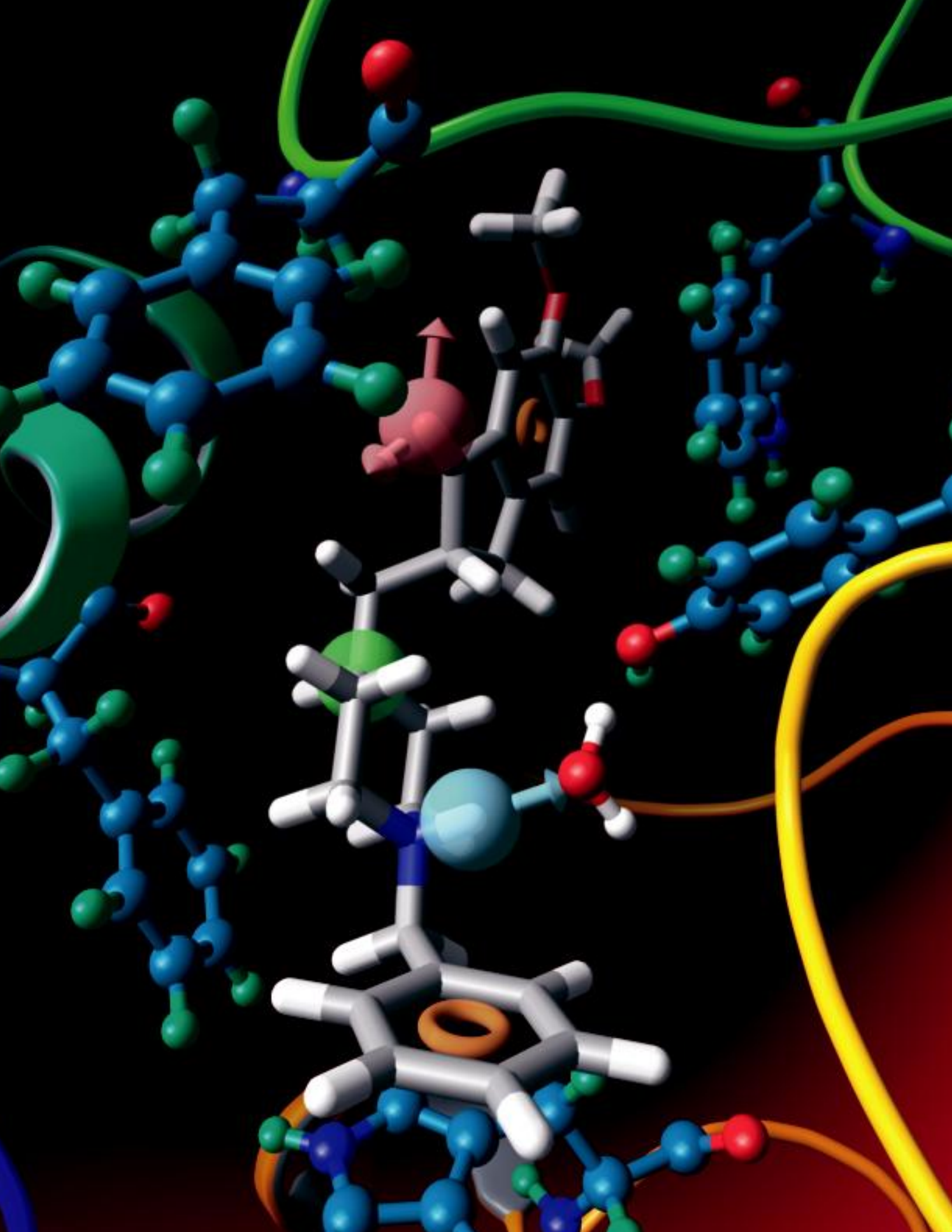
Maestro

A powerful, all-purpose molecular modeling environment

Maestro is the unified interface for all Schrödinger software. Impressive rendering capabilities, a powerful selection of analysis tools, and an easy-to-use design combine to make Maestro a versatile modeling environment for all researchers.

SCHRÖDINGER®



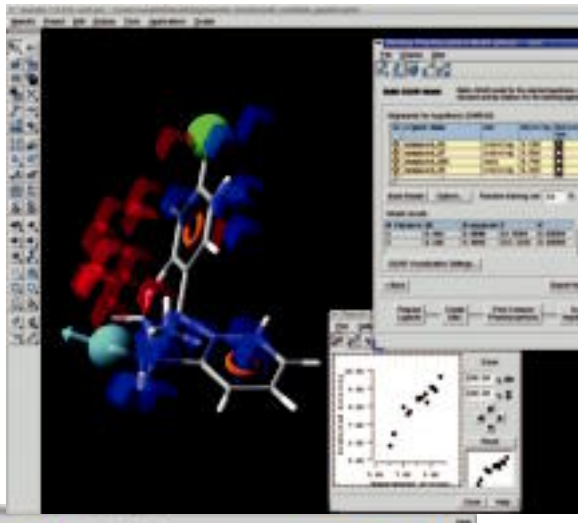
Maestro: Maximizing Returns in Computational Modeling

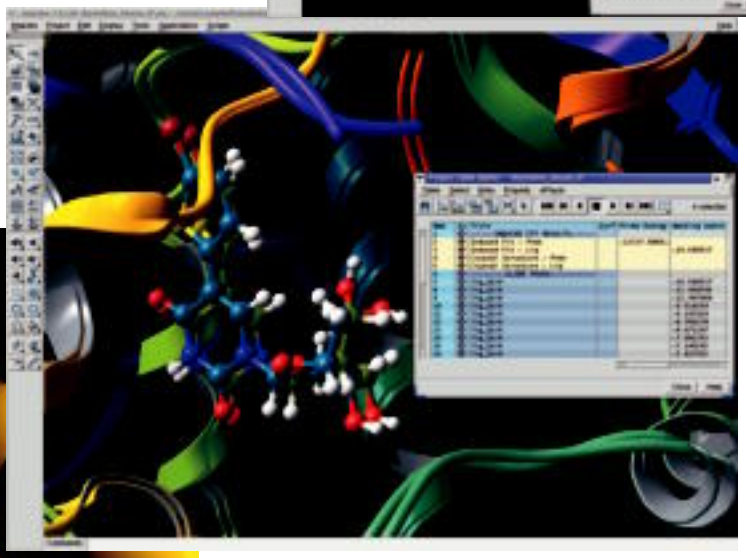
Schrödinger develops state-of-the-art chemical simulation software for use in pharmaceutical, biotechnology, and materials science research. Since its founding in 1990, Schrödinger has earned a reputation for its leadership in scientific development. Schrödinger's products range from general molecular modeling programs to a complete suite of drug design software including both ligand- and structure-based methods.

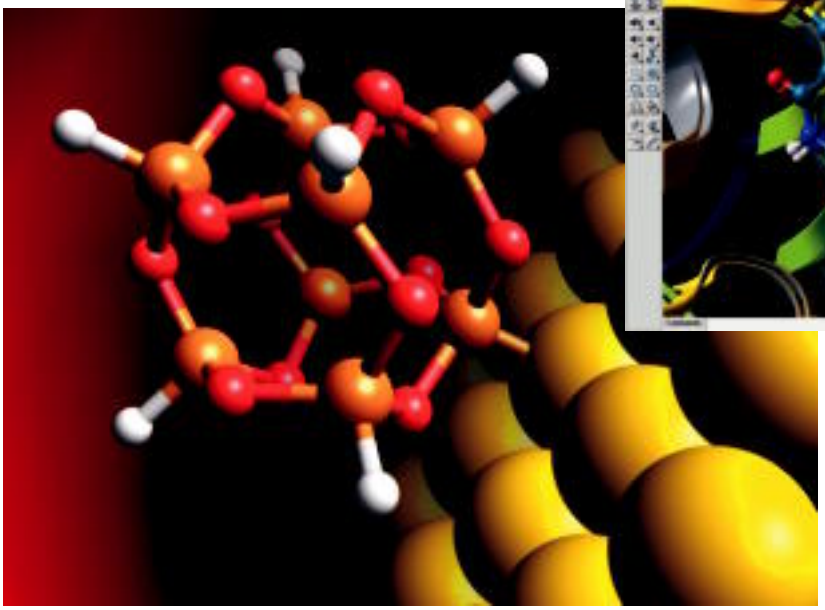
Maestro is the linchpin of Schrödinger's computational technology. Far more than just a visualization program, Maestro also helps researchers organize and analyze data. Maestro's intuitive interface makes setting up calculations easy and straightforward. Computed results are automatically returned and incorporated into projects for further study. Maestro's vast array of visualization options makes it possible to glean insight into molecular properties as well as detailed intermolecular interactions. Maestro is a powerful and versatile molecular modeling environment, and the portal to the most advanced science in computational chemistry.

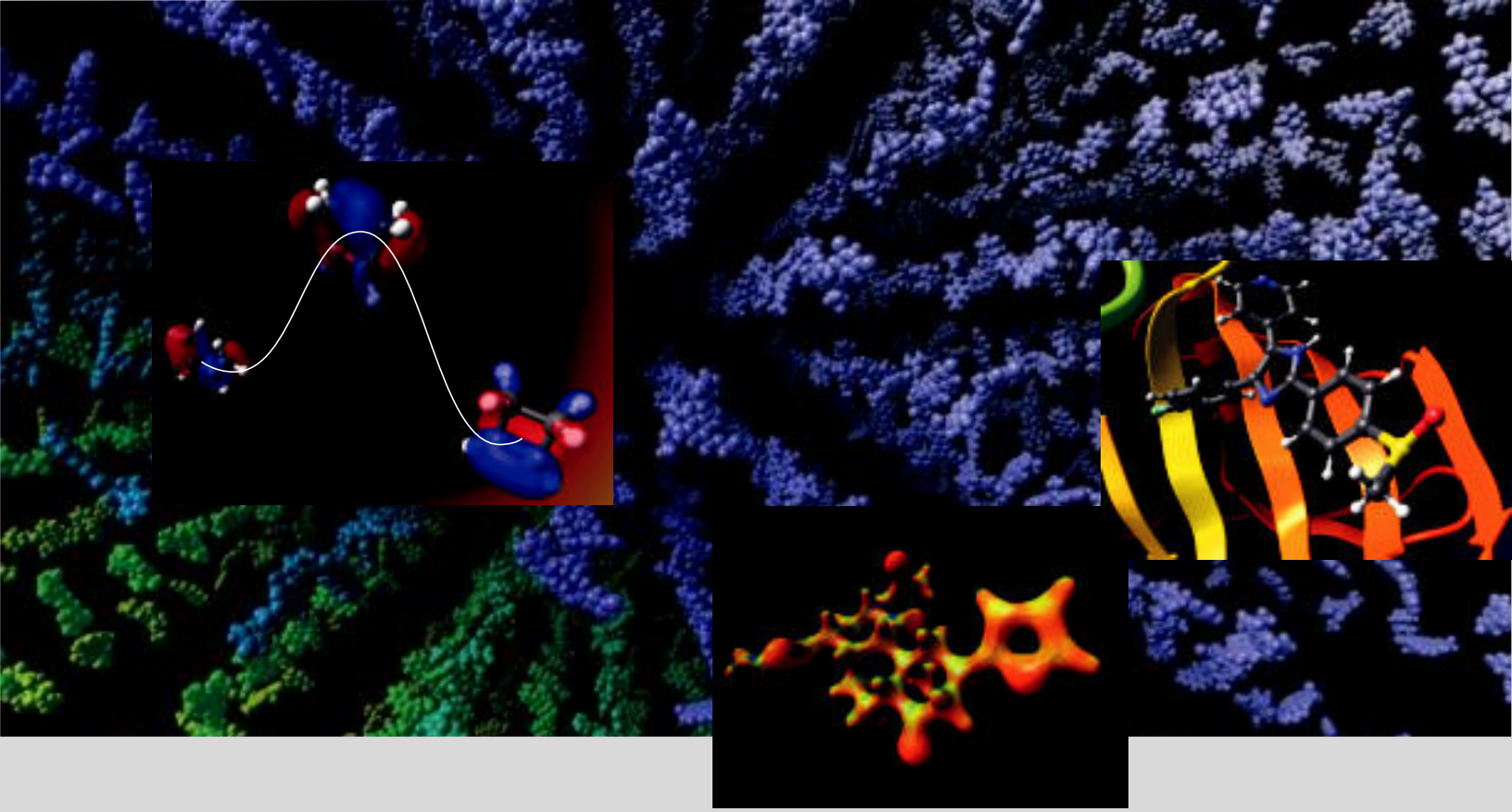
Designed to bring ease-of-use to powerful modeling technology, Maestro empowers its users with an impressive array of features:

- **Model generation:** Maestro supports many common file formats for structural input. In addition, Maestro provides an intuitive, full-featured building tool for constructing molecular models of any type.
- **Flexible visualization:** Maestro provides many viewing options to accommodate the varied needs of different applications. From small molecules to large biomolecular complexes, Maestro brings clarity to a wide range of modeled systems.
- **3D realism:** Maestro's superior rendering and stereographic capabilities allow researchers to view complex molecular systems as three-dimensional objects with unrivaled realism.









- **Quantitative structural analysis:** Maestro includes versatile measurement tools that give the user the ability to precisely quantify a molecule's structural features. Superimposition tools make possible detailed comparisons between structures.
- **Customization scripts:** Maestro offers the ability to customize and automate tasks as well as manage workflow via scripting. Rather than a proprietary language, Maestro scripts are written in the industry-standard Python language.
- **Molecular properties:** Computed properties such as vibrational modes, molecular orbitals, or electron density are easily visualized in Maestro. The unique Sitemap feature locates areas within a protein that correspond to hydrophobic or hydrophilic regions.
- **Unified interface:** Maestro is the common interface for all Schrödinger computational programs. This shared modeling environment makes it easy for novices and experts alike to set up computational studies without having to relearn a new interface.
- **Data management and analysis:** Maestro employs a data system that automatically archives structure-related properties. A built-in plotting facility helps elucidate structure-property relationships.
- **Publication and presentation:** Maestro outputs high-resolution, presentation-quality images that can be easily incorporated into documents for publication or for sharing data with colleagues.
- **Easy to use:** Maestro provides context-sensitive feedback and seamlessly guides the user through intuitive, step-by-step interfaces. Online help makes it possible to master the program with an abbreviated learning curve.
- **Continued development:** Maestro continues to evolve in usability through productivity enhancements such as toolbars, wizard-like interface, and most recently, Python scripting.
- **Cross-platform support:** In addition to offering excellent performance on Linux and SGI, Maestro can be displayed across a network to many commonly used platforms, including Windows and Mac.

Schrödinger Computational Technology

Schrödinger's state-of-the-art computational technology ranges from general molecular modeling to a complete suite of drug design software including both ligand- and structure-based methods. The individual products include:

Glide

Complete solution for ligand-receptor docking

Glide offers the full spectrum of speed and accuracy from high-throughput virtual screening of millions of compounds to extremely accurate binding mode predictions, providing consistently high enrichment at every level.

Jaguar

Rapid ab initio electronic structure calculation

Jaguar is a high-performance ab initio package for both gas and solution phase simulations, with particular strength in treating metal-containing systems, making it the most practical quantum mechanical tool for solving real-world problems.

Liaison

Efficient and accurate ligand-receptor binding free energy prediction

Liaison applies the linear interaction approximation to accurately compute binding affinities for series of ligands with similar binding modes, making it a powerful tool for lead optimization.

LigPrep

Versatile generation of accurate 3D molecular models

LigPrep goes far beyond simple 2D to 3D structure conversions by including tautomeric, stereochemical, and ionization variations, as well as energy minimization and flexible filters to generate fully customized ligand libraries that are optimized for further computational analyses.

MacroModel

Versatile, full-featured program for molecular modeling

MacroModel combines leading force fields, accurate solvation models, and advanced conformational searching methods to provide the most complete molecular modeling package with performance suitable for a wide range of research.

Phase

High-performance program for ligand-based drug design

Phase is a complete package of pharmacophore modeling tools that gives chemists an unparalleled level of control at each step. Fast, accurate, and highly configurable, Phase is a powerful tool for lead discovery and lead optimization.

Prime

Powerful and innovative package for accurate protein structure predictions

Prime intuitively guides chemists from a sequence alignment to a refined protein structure. Used in conjunction with Glide as part of Schrödinger's Induced Fit protocol, Prime quickly and accurately predicts the conformational changes induced by ligand binding.

QikProp

Rapid ADME predictions

QikProp efficiently evaluates a widely applicable set of pharmaceutically relevant properties at a rate of over half a million compounds per hour, making it an indispensable tool for applying ADME principles in lead discovery and optimization.

QSite

High-performance QM/MM program

QSite applies quantum mechanics to the reactive center of a protein active site and molecular mechanics to the rest of the system. Its accuracy allows detailed understanding of reactions involving proteins, making it a powerful tool for lead optimization.

Strike

Powerful software for statistical modeling and QSAR

Strike is a highly capable statistical modeling package designed especially for chemists. An easy-to-use interface and wide variety of tools combine to make Strike the software of choice for developing and applying quantitative structure-activity relationships.

Obtaining Copies

Maestro is provided at no charge with the purchase of any Schrödinger computational program. Visit the Schrödinger web site to download Maestro.

Maestro

A powerful, all-purpose molecular modeling environment

System Requirements:

LINUX
- Pentium or better
- Linux kernel 2.4 (Red Hat 7.3) or later
- 256 MB memory

SGI
- R5000 or better
- IRIX 6.5.2m or later
- 256 MB memory

Additional Information:

www.schrodinger.com
info@schrodinger.com

A Coordinated Family of Products

All Schrödinger products are seamlessly integrated through the Maestro graphical interface. Schrödinger has a full suite of software for drug design, including both structure- and ligand-based methods. For a full listing of all of Schrödinger's computational products, please refer to the inside cover.

120 West 45th Street
29th Floor
New York, NY 10036

101 SW Main Street
Suite 1300
Portland, OR 97204

3655 Nobel Drive
Suite 430
San Diego, CA 92122

Dynamostraße 13
68165 Mannheim
Germany

Quatro House, Frimley Road
Camberley GU16 7ER
United Kingdom

SCHRÖDINGER.